

LINEAR DAES WITH NONSMOOTH FORCING

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Abstract. State transfer functions are derived for linear time invariant differential-algebraic equations of arbitrary index subject to insufficient smoothness in the forcing functions. As a result, it is demonstrated that the problem of reinitialization after discontinuities is always fully and uniquely determined. Algorithmic implementations and extensions to the linear time varying and nonlinear cases are discussed.

Key words. differential-algebraic equations, hybrid systems, discontinuity, state transfer functions, high index

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1. Introduction. In recent years hybrid (discrete/continuous) dynamic systems that exhibit coupled continuous and discrete behavior have attracted much attention in a number of applications. Hybrid systems may be modeled by a variety of embedded differential or difference equations, and may exhibit several categories of discontinuous behavior at discrete points in time known as *events*, including nonsmooth forcing, switching of the vector field, and jumps in the state [2]. Here we will be concerned with a limited class of such systems where the embedded differential system is a single system of linear time invariant differential-algebraic equations (LTI DAEs) subject to nonsmoothness in the forcing only. We are primarily interested in an appropriate definition of solvability for such systems in the presence of nonsmooth forcing, and the resulting implications for simulation. This is related to what has become known as the problem of *reinitialization after discontinuities*: in the absence of an explicit specification of the state transfer, what subset of state variables should by default be treated as continuous across a discontinuity at an event? These state transfer functions may be used to formulate a consistent initialization calculation in order restart numerical integration immediately following the event.

Brüll and Pallaske [3] study classes of nonlinear index 1 DAEs, and in some cases are able to identify functions of the state variables that remain continuous at a discontinuity in the forcing functions, yielding fully determined consistent initialization problems. Majer *et al.* [14] also study classes of nonlinear index 1 DAEs and identify subsets of state variables that remain continuous, yielding either fully or under determined consistent initialization problems. Gopal and Biegler [13] consider LTI DAEs of arbitrary index subject to discontinuous forcing. They argue that the dependence of an underlying ODE (UODE) of the DAE on the derivatives of the forcing functions may be employed to identify which state variables are continuous at such discontinuities. In general this yields an under determined consistent initialization problem because the number of continuous state variables may be less than the degrees of freedom available. The key result of the present paper shows that in fact, for LTI DAEs of arbitrary index, this consistent initialization problem can be viewed as always fully and uniquely determined. One may conjecture that this observation extends to general nonlinear DAEs, but proof appears to be very difficult.

The problem considered is also related to the so-called distribution solution of linear DAEs [21, 6, 12, 18]. The typical approach is to consider that a DAE starts describing the system evolution at time $t = 0$, and that for $t < 0$ the state trajectory $\mathbf{x}(t)$ is arbitrary. Since there is no reason that $\lim_{t \rightarrow 0^-} \mathbf{x}(t)$ should be consistent with the DAE at $t = 0$, it is necessary to consider the existence and uniqueness of impulses at $t = 0$ that will “jump” the state to a consistent value. In this paper

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we are concerned with an initial value problem described by a single DAE system that starts from a consistent initial condition, but then experiences insufficient smoothness in the forcing at later points in time. Thus we ask: how is the state transferred at these points? In [19] a comprehensive existence and uniqueness theory is developed for linear DAEs with discontinuous forcing when the coefficient matrices are smooth functions of time. This theory encompasses the LTI case considered below. Indeed, these authors remark that, at least in principle, there is a unique and calculable jump in the state at a discontinuity in the forcing [19][Remark 3.5]. In closing, they develop highly tailored numerical algorithms for the index 1 and index 2 cases (only), based on the ‘reduction procedure’ also employed for their theoretical development.

In light of this earlier work, the present paper makes the following contributions. First, in the linear time invariant case we develop an alternative and much simpler theory. It is hoped that our analysis will be more accessible to the community interested in computation. Indeed, it is closely related to the widely adopted notion of reinitialization after discontinuities discussed above. Moreover, our analysis may be readily extended to a quite general class of linear time varying (LTV) DAEs and certain nonlinear DAEs. Finally, our analysis prompts the development of a computational approach that can be applied to large-scale sparse systems of arbitrary index. This approach can be used in conjunction with any numerical integration and event location algorithms suitable for the index and degree of nonlinearity in question.

2. Analysis. Consider the LTI DAE:

$$\mathbf{A}\dot{\mathbf{x}}(t) + \mathbf{B}\mathbf{x}(t) = \mathbf{f}(t) \quad (2.1)$$

where $\mathbf{A}, \mathbf{B} \in \mathcal{L}(\mathbb{R}^n, \mathbb{R}^n)$ are $n \times n$ matrices, $\mathbf{f} : I \rightarrow \mathbb{R}^n$ and $I = [t_0, t_f]$. \mathbf{A} is singular. Classical notions of solvability on I (e.g., [4]) require for every admissible $\mathbf{f}(t)$ there exists at least one continuously differentiable solution $\mathbf{x}(t)$, and that all solutions for a particular $\mathbf{f}(t)$ are defined on all of I , are at least continuously differentiable, and are uniquely determined by their (assumed consistent) value at any $t \in I$. This will require assumptions concerning sufficient differentiability of $\mathbf{f}(t)$ on I ; it is immediately evident that some or all elements of $\mathbf{f}(t)$ will have to be at least continuously differentiable.

Here we are concerned with problems in which the elements of $\mathbf{f}(t)$ are sufficiently differentiable on I except at a finite set of distinct points in time $E = \{t_i \in (t_0, t_f) : t_{i-1} < t_i, i = 1 \dots n_e\}$ (events). Clearly at events some or all elements of \mathbf{x} will not be defined. Let $I^s = I \setminus E$ and $t_f = t_{n_e+1}$. We then define solvability of the DAE (2.1) with nonsmooth forcing on I to require that for every such nonsmooth $\mathbf{f}(t)$ there exists at least one continuously differentiable solution $\mathbf{x}(t)$ on I^s , and that all solutions for a particular $\mathbf{f}(t)$ are defined on all of I^s , are at least continuously differentiable on I^s , and are uniquely determined by their (assumed consistent) value at any $t \in I^s$. This definition seems most consistent with modern algorithms employed for simulation of hybrid systems (e.g., [17]).

A necessary condition for solvability with nonsmooth forcing is that the pencil $\lambda\mathbf{A} + \mathbf{B}$ is regular, which implies there will exist nonsingular matrices \mathbf{P}, \mathbf{Q} such that [11]:

$$\mathbf{P}\mathbf{A}\mathbf{Q} = \begin{bmatrix} \mathbf{I} & \mathbf{0} \\ \mathbf{0} & \mathbf{N} \end{bmatrix} \quad \mathbf{P}\mathbf{B}\mathbf{Q} = \begin{bmatrix} \mathbf{C} & \mathbf{0} \\ \mathbf{0} & \mathbf{I} \end{bmatrix} \quad (2.2)$$

\mathbf{N} has nilpotency ν (the index of the DAE) and suppose the first block contains r rows (the degrees of freedom for consistent initialization). Defining the new variables $\mathbf{x} = \mathbf{Q}\mathbf{y}$ and premultiplying by \mathbf{P} yields:

$$\dot{\mathbf{y}}_1 + \mathbf{C}\mathbf{y}_1 = \mathbf{g}_1(t) \quad (2.3)$$

$$\mathbf{N}\dot{\mathbf{y}}_2 + \mathbf{y}_2 = \mathbf{g}_2(t) \quad (2.4)$$

The elements of \mathbf{g}_1 , \mathbf{g}_2 are linear combinations of the elements of \mathbf{f} . The solution of this system is evident from inspection [11, 22]:

$$\mathbf{y}_1(t) = \exp(-\mathbf{C}(t - t_0))\mathbf{y}_1(0) + \int_{t_0}^t \exp(-\mathbf{C}(t - \tau))\mathbf{g}_1(\tau)d\tau \quad (2.5)$$

$$\mathbf{y}_2(t) = \sum_{j=0}^{\nu-1} (-1)^j \mathbf{N}^j \mathbf{g}_2^{(j)} \quad (2.6)$$

Sufficient differentiability for the forcing functions on I^s may be deduced directly from this solution. It is also evident that existence and uniqueness of $\mathbf{y}_1(t)$ is entirely related to existence of the integral in (2.5), and $\mathbf{y}_2(t)$ is uniquely defined on I^s . At the events t_i some or all elements of \mathbf{f} do not satisfy the sufficient differentiability requirements, so some or all elements of \mathbf{y}_2 will be undefined. It is possible to characterize \mathbf{y}_2 at the events more precisely in terms of distributions [19], but this is largely irrelevant for simulation. Nevertheless, both $\lim_{t \rightarrow t_i^-} \mathbf{y}_2$ and $\lim_{t \rightarrow t_i^+} \mathbf{y}_2$ are uniquely defined. Similarly, impulsive forcing at events will imply some or all elements of \mathbf{y}_1 are undefined, but the left and right limits are uniquely defined. Identical conclusions may be reached via an analysis in the frequency domain (e.g., [21, Eqns. (12ab)]).

The issue of reinitialization after discontinuities may now be addressed. Assuming existence of the integral, in the absence of impulsive forcing it is evident from inspection of (2.5–2.6) that \mathbf{y}_1 should be treated as continuous at events. Moreover, the dimension of \mathbf{y}_1 equals the degrees of freedom available for consistent initialization, so these continuity conditions fully define $\lim_{t \rightarrow t_i^+} \mathbf{y}$ in terms of $\lim_{t \rightarrow t_i^-} \mathbf{y}$. Rewriting the change of variables as:

$$\begin{bmatrix} \mathbf{y}_1 \\ \mathbf{y}_2 \end{bmatrix} = \begin{bmatrix} \mathbf{Q}_1^{-1} \\ \mathbf{Q}_2^{-1} \end{bmatrix} \mathbf{x} \quad (2.7)$$

reveals that in the original space the state transfer amounts to continuity of certain linear combinations of \mathbf{x} :

$$\mathbf{Q}_1^{-1} \mathbf{x}(t_i^+) = \mathbf{Q}_1^{-1} \mathbf{x}(t_i^-) \quad (2.8)$$

In the presence of impulsive forcing the state transfer is modified to include a contribution from the integral of the distributions. Once this ‘default’ state transfer is known, sensitivity analysis of such problems can also be performed, along the lines described in [10].

In [2] the term jump or impulse is adopted for the class of hybrid phenomena where the differential state $\mathbf{x}(t)$ is discontinuous at events. If the continuous dynamics are described by an ODE system, such jumps correspond identically to impulsive forcing. Inspection of (2.6) reveals that in the general case higher order discontinuities in the forcing functions may cause the state to jump. Defining a jump as $\Delta \mathbf{x}(t_i) = (\lim_{t \rightarrow t_i^+} \mathbf{x} - \lim_{t \rightarrow t_i^-} \mathbf{x})$ and rewriting the change of variables yields:

$$\Delta \mathbf{x}(t_i) = \mathbf{Q}_3 \Delta \mathbf{y}_1(t_i) + \mathbf{Q}_4 \Delta \mathbf{y}_2(t_i) \quad (2.9)$$

i.e., the relevant columns of \mathbf{Q} form bases for *impulsive* and *nonimpulsive* subspaces respectively. A move in the impulsive subspace \mathbf{Q}_3 may only be implemented via impulsive forcing, whereas a move in the *nonimpulsive* subspace \mathbf{Q}_4 may only be implemented by a step change or sometimes higher order discontinuity (i.e., impulsive forcing will not alter $\Delta \mathbf{y}_2(t_i)$). Together, these subspaces span \mathbb{R}^n , so provided the forcing affects all elements of \mathbf{y} , an arbitrary jump may be implemented with a suitable combination of discontinuities of the appropriate order.

3. Example. Consider the DAE ($\nu = 1, r = 1$) [1]:

$$\begin{bmatrix} 1 & 2 \\ 0 & 0 \end{bmatrix} \dot{\mathbf{x}} + \begin{bmatrix} 0 & 0 \\ 1 & 1 \end{bmatrix} \mathbf{x} = \begin{bmatrix} 0 \\ f(t) \end{bmatrix} \quad (3.1)$$

The Gauss-Jordan analysis proposed by Gopal and Biegler [13] yields the UODE:

$$\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \dot{\mathbf{x}} + \begin{bmatrix} 0 & 0 \\ 0 & 0 \end{bmatrix} \mathbf{x} = \begin{bmatrix} 2f'(t) \\ -f'(t) \end{bmatrix} \quad (3.2)$$

which correctly indicates that both elements of \mathbf{x} will jump in response to a discontinuity in $f(t)$. The canonical form for this system is:

$$\begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix} \dot{\mathbf{y}} + \begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix} \mathbf{y} = \begin{bmatrix} 0 \\ -f(t) \end{bmatrix}, \quad \mathbf{Q} = \begin{bmatrix} -1 & -2 \\ 1 & 1 \end{bmatrix} \quad (3.3)$$

which indicates:

$$y_1 = x_1 + 2x_2 \quad (3.4)$$

$$y_2 = -x_1 - x_2 \quad (3.5)$$

and that at a discontinuity in $f(t)$ both elements of \mathbf{x} will jump, but the following linear combination will remain continuous across the event:

$$x_1(t_i^+) + 2x_2(t_i^+) = x_1(t_i^-) + 2x_2(t_i^-) \quad (3.6)$$

uniquely defining the consistent reinitialization problem. This result may also be obtained via the analysis of Brüll and Pallaske [3], but the present work extends to LTI DAEs of arbitrary index and dimension.

The impulsive and nonimpulsive subspaces are spanned by $[-1, 1]^T$ and $[-2, 1]^T$ respectively. For the forcing specified, only jumps in the nonimpulsive subspace are possible, and these are implemented by step changes.

4. Computation. The practical implementation of the above results is complicated by the inherent instability of computing the canonical form [7].

4.1. Direct Approach. On the other hand, the generalized upper triangular form of a matrix pencil may be computed stably via unitary transformations [7]. Suppose we begin with the conjugate transpose of the matrix pencil in (2.1), $\mathbf{B}^H - \lambda\mathbf{A}^H$. There exist unitary matrices \mathbf{P}, \mathbf{Q} such that:

$$\mathbf{P}^H(\mathbf{B}^H - \lambda\mathbf{A}^H)\mathbf{Q} = \mathbf{U} \quad (4.1)$$

where \mathbf{U} is upper triangular (its diagonal entries are related to the generalized eigenvalues). Taking the conjugate transpose of both sides yields:

$$\mathbf{Q}^H\mathbf{B}\mathbf{P} - \lambda\mathbf{Q}^H\mathbf{A}\mathbf{P} = \mathbf{L} \quad (4.2)$$

where \mathbf{L} is lower triangular and the diagonal entries are unchanged. This demonstrates that unitary matrices exist that will transform any matrix pencil to a generalized lower triangular form.

Now suppose that \mathbf{P} and \mathbf{Q} have been chosen so that the terms related to the $n - r$ infinite generalized eigenvalues appear as the final $n - r$ entries on the diagonal of \mathbf{L} . It is then evident that the first r rows of \mathbf{L} correspond to a differential part that is decoupled from the algebraic part of the problem. For the purposes of reinitialization after discontinuities, these r transformed variables may be treated as continuous, yielding the same result as the fully decoupled canonical form.

The subroutine GUPTRI [8], for example, performs all the necessary calculations. Conveniently, if the pencil is regular, the generalized eigenvalues are arranged down the diagonal in the order: zero eigenvalues, then nonzero eigenvalues, and then infinite eigenvalues. When GUPTRI is applied to the conjugate transpose of (3.1) it yields:

$$\mathbf{P} = \begin{bmatrix} -1/\sqrt{5} & 2/\sqrt{5} \\ -2/\sqrt{5} & -1/\sqrt{5} \end{bmatrix} \quad \mathbf{Q} = \mathbf{I} \quad (4.3)$$

The first and second rows correspond to a zero and an infinite eigenvalue respectively. From inspection of the conjugate transpose of \mathbf{P} we conclude that the linear combination $-(1/\sqrt{5})x_1 - (2/\sqrt{5})x_2$ should remain continuous at discontinuities in the forcing. This is identical to the conclusion drawn above.

A drawback of this direct approach is that the operations involved in computing the generalized upper triangular form are inherently dense. This limits its extension to sparse, large-scale problems, although this is somewhat mitigated by the fact that the linear transformation only needs to be computed once during the course of a simulation.

4.2. Indirect Approach. Pantelides [16] describes a graph-theoretical algorithm that aims to identify subsets of equations, the differentiation of which yields additional ‘hidden’ constraints on the consistent initial conditions of a DAE. It is well known that this ‘structural’ approach may potentially yield too few [16] or too many extra equations [20]. Suppose that this algorithm performs correctly as intended when applied to (2.1) (in our experience, this is a very common occurrence with physical models). The method of dummy derivatives [15] may then be applied to derive a larger index one DAE with an equivalent solution set. This is achieved by substituting a subset of the time derivatives appearing in the over determined system formed from augmenting the hidden constraints to (2.1) with dummy algebraic variables (assume that additional variables and equations are introduced as necessary to retain a first order system). The resulting system is fully determined and index one. Label the subset of variables whose time derivatives appear in the equivalent index one system \mathbf{z} , and those variables that only appear algebraically \mathbf{y} . By construction, there will exist elementary row operations that transform the equivalent index one DAE to:

$$\begin{bmatrix} \mathbf{I} & \mathbf{0} \\ \mathbf{H}_1 & \mathbf{H}_2 \end{bmatrix} \begin{bmatrix} \dot{\mathbf{z}} \\ \mathbf{y} \end{bmatrix} + \begin{bmatrix} \mathbf{D}_1 \\ \mathbf{D}_2 \end{bmatrix} \mathbf{z} = \mathbf{g}(t) \quad (4.4)$$

where \mathbf{z} has dimension r and \mathbf{g} may involve derivatives of elements of \mathbf{f} . The only assumption required for this transformation is that Pantelides’ algorithm has performed correctly as intended. In addition, all required operations can exploit sparsity in large-scale problems [9]. Insufficient smoothness may introduce distributions on the right hand side of the first block row of (4.4). However, due to the identity on the left hand side, it is easy to evaluate the integral across the event, and hence define state transfer functions for \mathbf{z} .

Consider again (3.1). Application of the indirect procedure differentiates the second equation once, yielding two alternative equivalent index one systems, one of which is:

$$\begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 1 & 0 & 1 \end{bmatrix} \begin{bmatrix} \dot{x}_2 \\ x_1 \\ x'_1 \end{bmatrix} + \begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix} x_2 = \begin{bmatrix} -f'(t) \\ f(t) \\ f'(t) \end{bmatrix} \quad (4.5)$$

where x'_1 is the dummy algebraic variable that replaces \dot{x}_1 . Suppose that $f(t) = H(t)$ (the Heaviside function), which implies $f'(t) = \delta(t)$ and $\Delta x_2(0) = -\int_0^0 \delta(t) dt = -1$. From the second row it follows that:

$$\Delta x_1(0) + \Delta x_2(0) = 1 \quad (4.6)$$

which implies $\Delta x_1(0) = 2$, and $\Delta x_1(0) + 2\Delta x_2(0) = 0$, as would be expected (3.6).

Note that Pantelides' algorithm may be replaced in this procedure with any other suitable algorithm, perhaps one with stronger correctness properties.

4.3. Linear Time Varying DAEs. Consider the LTV DAE:

$$\mathbf{A}(t)\dot{\mathbf{x}} + \mathbf{B}(t)\mathbf{x} = \mathbf{f}(t) \quad (4.7)$$

where $\mathbf{A}(t)$ and $\mathbf{B}(t)$ are analytic. If this system is solvable, there will exist analytic $\mathbf{P}(t)$ and $\mathbf{Q}(t)$ that will transform (4.7) into Standard Canonical Form (SCF) [5]:

$$\dot{\mathbf{y}}_1 + \mathbf{C}(t)\mathbf{y}_1 = \mathbf{g}_1(t) \quad (4.8)$$

$$\mathbf{N}(t)\dot{\mathbf{y}}_2 + \mathbf{y}_2 = \mathbf{g}_2(t) \quad (4.9)$$

The state transfer functions are time varying and evident from the SCF. The utility of this result is limited by the fact that, in general, freezing the coefficient matrices at an event and computing either the canonical form or the generalized lower triangular form for the corresponding LTI DAE does not yield correct conclusions concerning the state transfer functions.

4.4. Nonlinear DAEs. Consider the nonlinear DAE:

$$\mathbf{A}\dot{\mathbf{x}} + \mathbf{h}(\mathbf{x}, t) = \mathbf{f}(t) \quad (4.10)$$

with nonsmoothness in the right hand side (only). The indirect approach may also be applied to this system, subject to the same assumption concerning the performance of Pantelides' algorithm. Because this system is linear in the derivatives, the equivalent index one system can always be transformed to one that has r equations explicit in $\dot{\mathbf{z}}$. However, it is important to note that elimination of \mathbf{y} from this first block row may involve nontrivial operations, and in general cannot even be carried out symbolically. Note also that in both the linear and nonlinear cases, r may equal zero, in which case there are no state transfer functions.

Consider the forced pendulum example in [13]. Application of the indirect approach yields two equivalent index one systems, one of which may be manipulated to (if $x \neq 1$; $u(t)$ is the forcing function):

$$\begin{aligned} \dot{x} &= v \\ \dot{v} &= \left(\pm u(t)\sqrt{1-x^2} - v^2 - \frac{x^2 v^2}{1-x^2} \right) x \\ y' &= w \\ w' &= -Ty - u(t) \\ x^2 + y^2 &= 1 \\ 2x\dot{x} + 2yy' &= 0 \\ 2\dot{x}^2 + 2x\dot{v} + 2y'^2 + 2yw' &= 0 \end{aligned} \quad (4.11)$$

Whilst this analysis does indicate that x and v should be treated as continuous, it leaves an ambiguity concerning the sign of y , and the value of all the related variables, including \dot{v} . In this case, the analysis of Gopal and Biegler [13] might be preferable because it would solve an over determined problem in which x , y , v and w are all treated as continuous. On the other hand, Gopal and Biegler's approach yields an ambiguity if linear combinations of the state variables should be treated as continuous. Formulation of an over determined problem where the requisite state transfer functions

together with any state continuity conditions from Gopal and Biegler are solved simultaneously with the equivalent index 1 system appears most appropriate in this case.

Extension of these ideas to more general nonlinear forms appears highly problematic. Consider the nonlinear index one example of Brüll and Pallaske [3]:

$$\begin{aligned} \dot{x}_1 + x_3 \dot{x}_2 &= 0 \\ x_2 &= u_1(t) \\ x_3 &= u_2(t) \end{aligned} \tag{4.12}$$

where $u_1(t) = u_2(t) = H(t)$. Elimination of x_3 using the third equation yields the LTV DAE:

$$\begin{aligned} \dot{x}_1 + u_2(t) \dot{x}_2 &= 0 \\ x_2 &= u_1(t) \end{aligned} \tag{4.13}$$

The current existence and uniqueness theory [19] does not cover the case where $u_2(t)$ is nonsmooth at an event. If we consider the left and right limits of the event, there is a discontinuity in the $\mathbf{P}(t)$ and $\mathbf{Q}(t)$ that transform this system to SCF. This suggests that this problem might be more akin to a switching in the vector field.

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